Lab 4- User Manual

Green Team

12/2/13

Version 1

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Introduction (Michael Rajs)

Allocated Resource Management Services (ARMS) configures a distributed resource management system, Sun Grid Engine, to handle resources on a cluster. The cluster being used is going to be modified on a research website application called Dinosolve. Dinosolve is a disulfide bond predictor that is important to scientists and researchers all over world because it helps them speed up their research to create new cures for diseases, new bioenergy, and new drug designs for pharmaceutical companies. In this user guide you will find helpful steps on how to register as a user, how to submit a sequence, how to login as a user, or administrator, and how to navigate easily through the Dinosolve website. The user guide will also help you in using and viewing special features associated with being a user, or an administrator.

Startup Screen (Jordan Heinrichs)

The start-up screen is the first thing you see when you open up the website (Figure 1). It can be loaded from any number of browsers such as Firefox, Google Crome, or even Internet Explorer. The page has a user friendly scrolling ability and the display is designed to fit any computer monitor. The start-up page contains a register button and a log in button that are located at the top right of the page (Figure 2).

When the register button is clicked a person will be redirected to a separate page and allowed to register to be a Dinosolve User. When the log in button is clicked a person will be redirected to a separate page allowed to log in as a Dinosolve user. The start-up page contains five buttons named Information, References, Statistics, Help and Contact which are located in the center of the page right below the logo (Figure 3). These buttons provide general and helpful information for the user to click on and view. For instance the “Information” tab will provide

general information about Dinosolve provided in Figure 4. The “Reference” tab provides information of how Dinosolve was implemented (Figure 5).

The “Statistics” tab describes and shows the accurate statistics of Dinosolve (Figure 6). The “Help” tab is a set be step explanation of how to use Dinosolve (Figure 7). And the “Contact” tab lets the user email and view the major contributors that helped to create Dinosolve (Figure 8). Below the five buttons are specific text fields named Title, Sequence, and Email and which are the required fields that must be filled out in order for a disulfide bond sequence to be processed, then solved and emailed to the user (Figure 9).

Figure 1. Startup Page

To register or login to the site simply click the “Register” or “Login” word located in red.

Figure 2. Startup Page Register and Login

To access Information, References, Statistics, Help, or Contact information click on the respective tabs located in the red box.

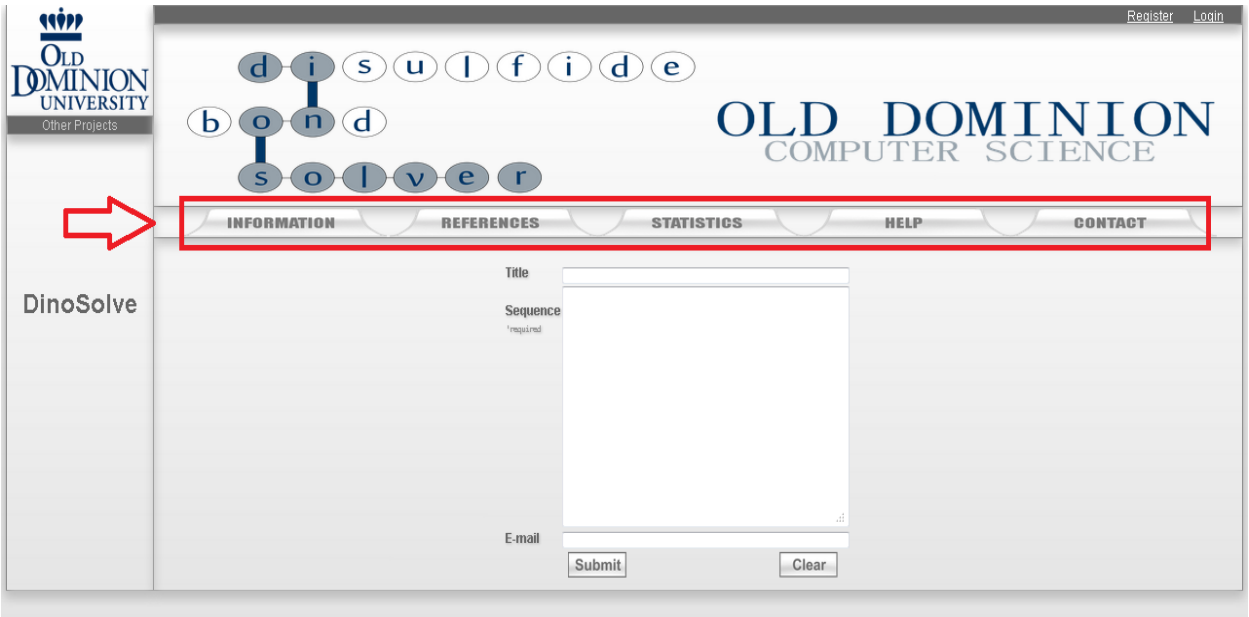

Figure 3. Startup Page Tabs

Register
Login
OLD DOMINION UNIVERSITY
Other Projects
disulfide bond solver
OLD DOMINION
COMPUTER SCIENCE
INFORMATION
REFERENCES
STATISTICS
HELP
CONTACT
DinoSolve
In this work, we introduce an approach of enhancing disulfide bonding prediction accuracy. We firstly derive the first-order and second-order mean-field potentials according to the amino acid environment around cysteine residues from large number of cysteine samples. The mean-field potentials are integrated as context-based scores to estimate the favorability of a cysteine residue in disulfide bonding state as well as a cysteine pair in disulfide bond connectivity.
These context-based scores are then incorporated as features together with other sequence and evolutionary information to train neural networks for disulfide bonding state prediction and connectivity prediction. Our computational results have shown that the context-based scores are effective features to enhance the prediction accuracies of both disulfide bonding state prediction and connectivity prediction. The 10-fold cross validated accuracy is 90.8% at residue-level and 85.6% at protein-level in classifying an individual cysteine residue as bonded or free, which is around 2% accuracy improvement. The average accuracy for disulfide bonding connectivity prediction is also improved, which yields overall sensitivity of 73.42% and specificity of 91.61%

Figure 4. Startup Information Tab

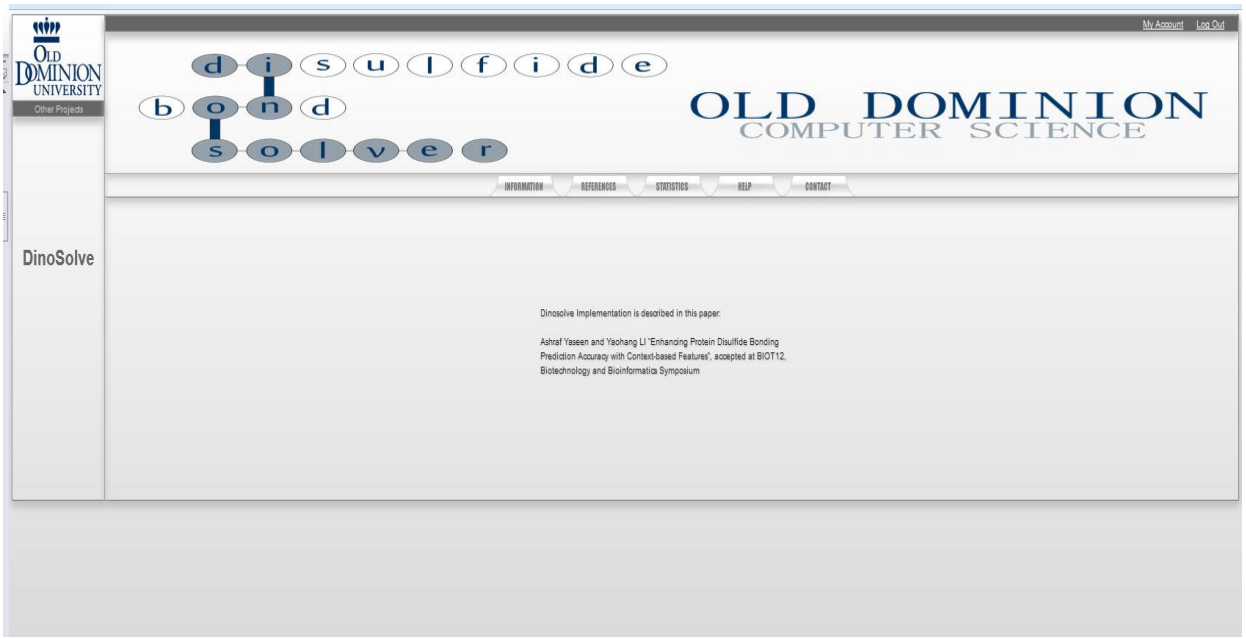

Figure 5. Startup Reference Tab

Figure 6. Startup Statistics Tab

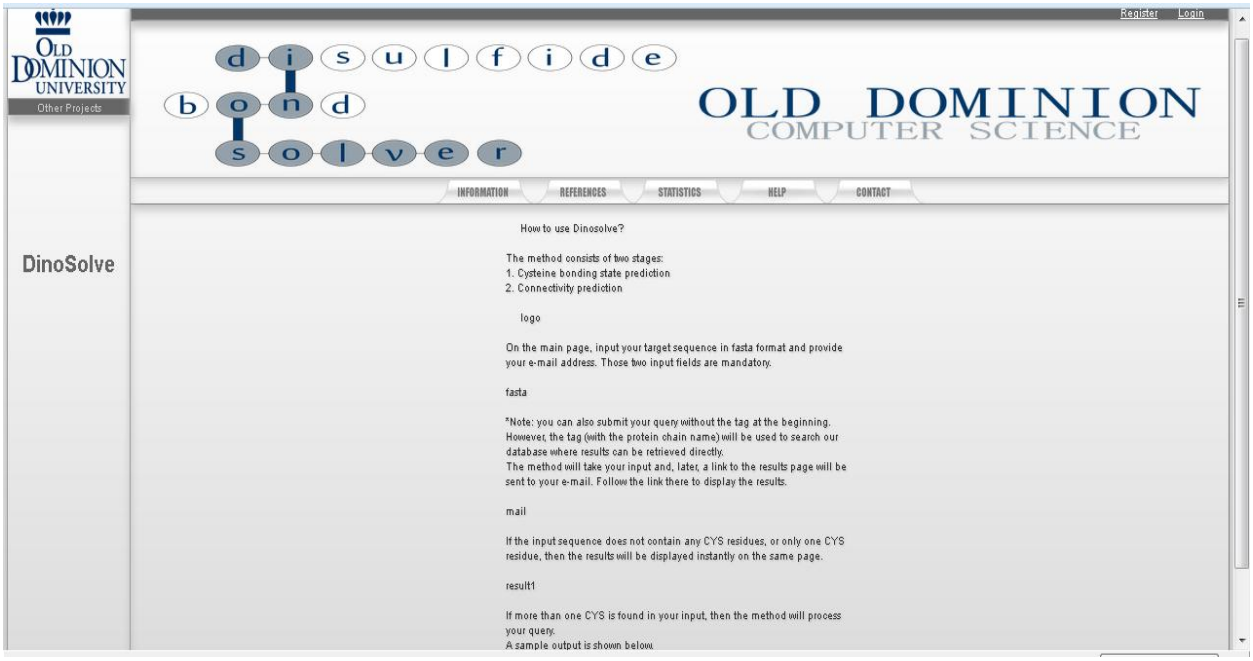
Register
Login
OLD DOMINION UNIVERSITY
Other Projects
disulfide bond solver
OLD DOMINION
COMPUTER SCIENCE
INFORMATION
REFERENCES
STATISTICS
HELP
CONTACT
DinoSolve
How to use Dinosolve?
The method consists of two stages:
1. Cysteine bonding state prediction
2. Connectivity prediction
logo
On the main page, input your target sequence in fasta format and provide your e-mail address. Those two input fields are mandatory.
fasta
*Note: you can also submit your query without the tag at the beginning. However, the tag (with the protein chain name) will be used to search our database where results can be retrieved directly.
The method will take your input and, later, a link to the results page will be sent to your e-mail. Follow the link there to display the results.
mail
If the input sequence does not contain any CYS residues, or only one CYS residue, then the results will be displayed instantly on the same page.
result1
If more than one CYS is found in your input, then the method will process your query.
A sample output is shown below.

Figure 7. Startup Help Tab

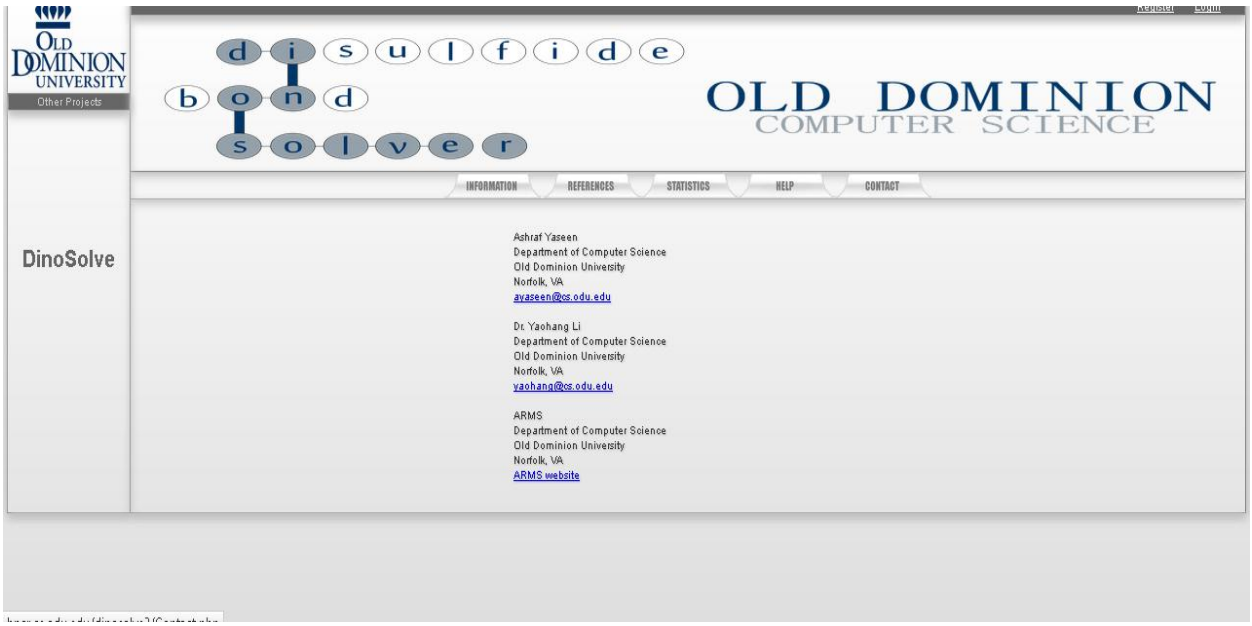

Figure 8. Startup Contact Tab

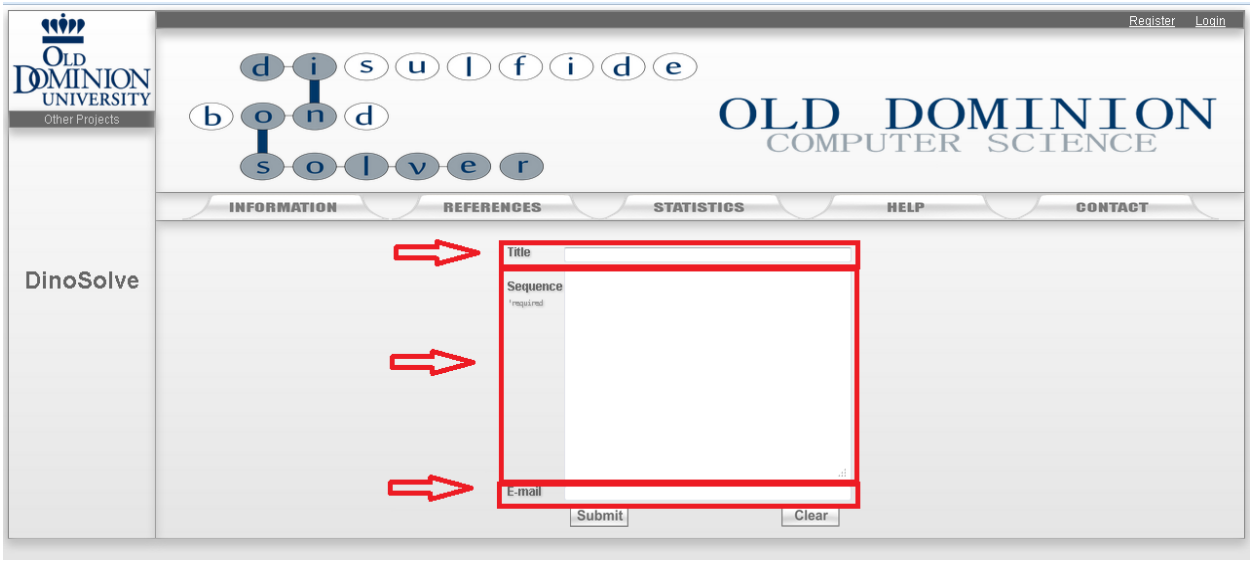

Figure 9. Startup Sequence Text Forms

Unregistered User (Adam Willis)

Submitting a sequence:

1. Input a title for your sequence in the box labeled “Title”. This is optional.

2. Input a sequence in the box labeled “Sequence”. Sequence must be 40 characters long and contain two cysteine residues.

3. Input your email address in the box labeled “E-mail”. This is how you will receive a link to the prediction results.

4. Click submit.

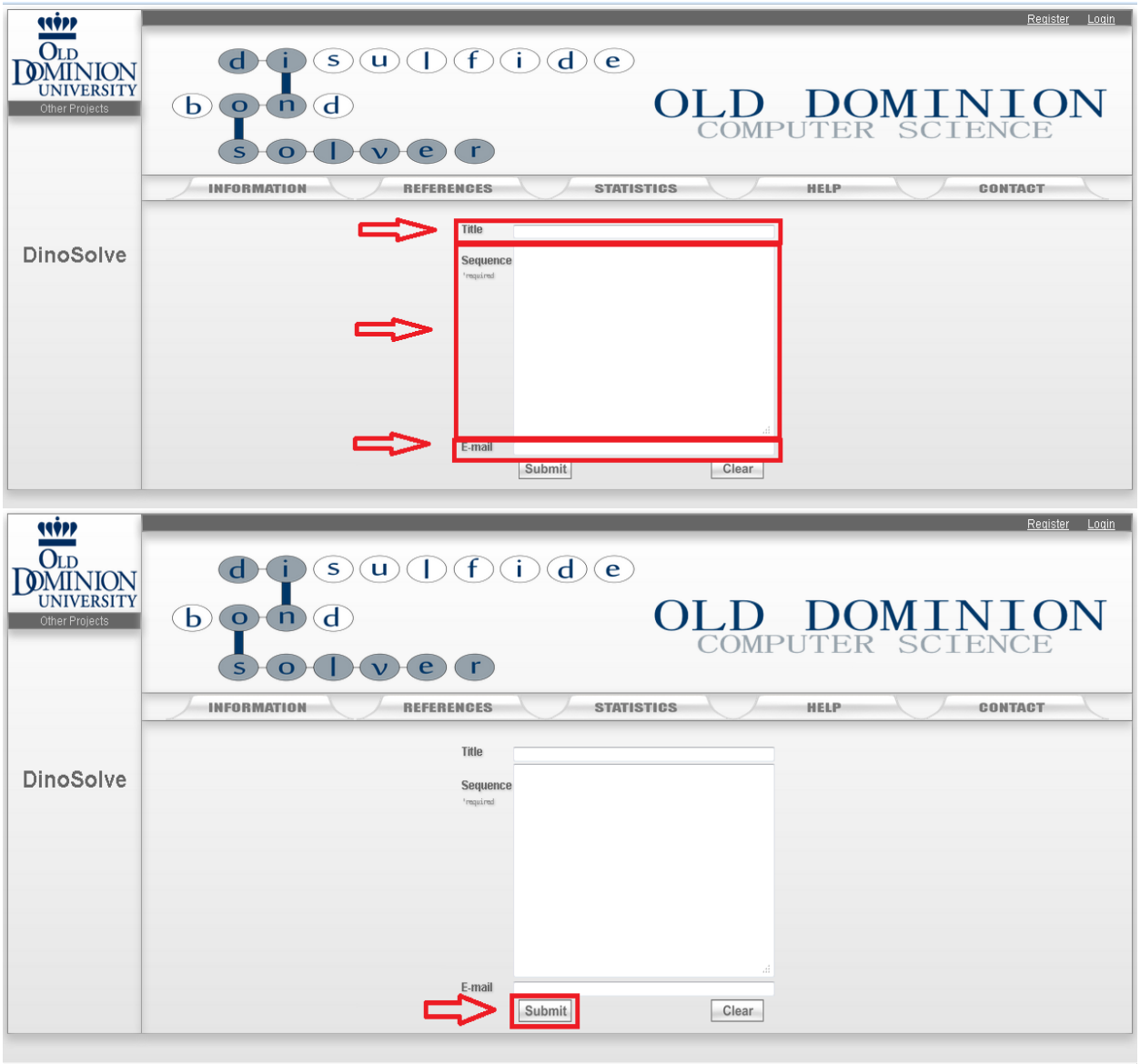

Figure 10. Unregistered User Submit Button

Viewing Prediction Results

1. You will receive an email with a link confirming your prediction results are ready.

2. Click the link to view your results.

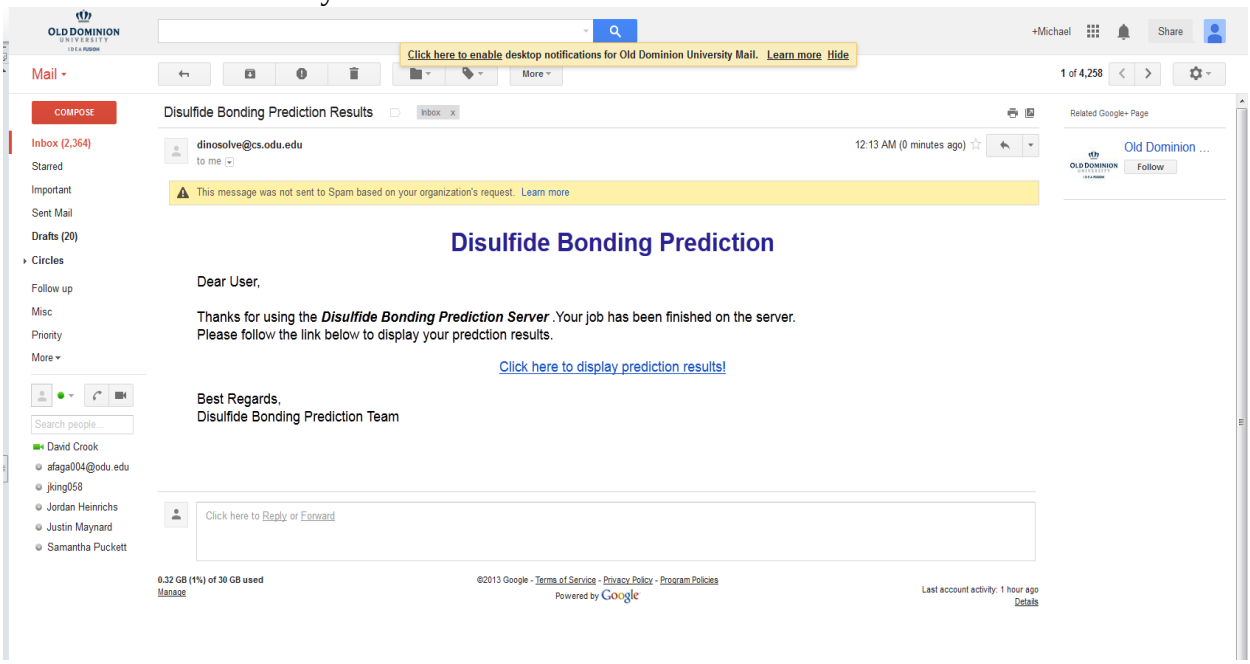

Figure 11. Email and Solution Link

How to Register as a User (Scott Pardue)

The register user screen located in figure 15 will provide a drop down box for you to provide your location. Right below that, there is a series of text boxes named email, password, and confirm password that you will need to fill out to become a registered user for Dinosolve (Figure 15). Once you fill out everything, click the “Submit” button located below the text boxes to be processed into the database as a user. If you just want to clear the form you can click the “Clear” button located to the right of the “Submit” button (Figure 16).

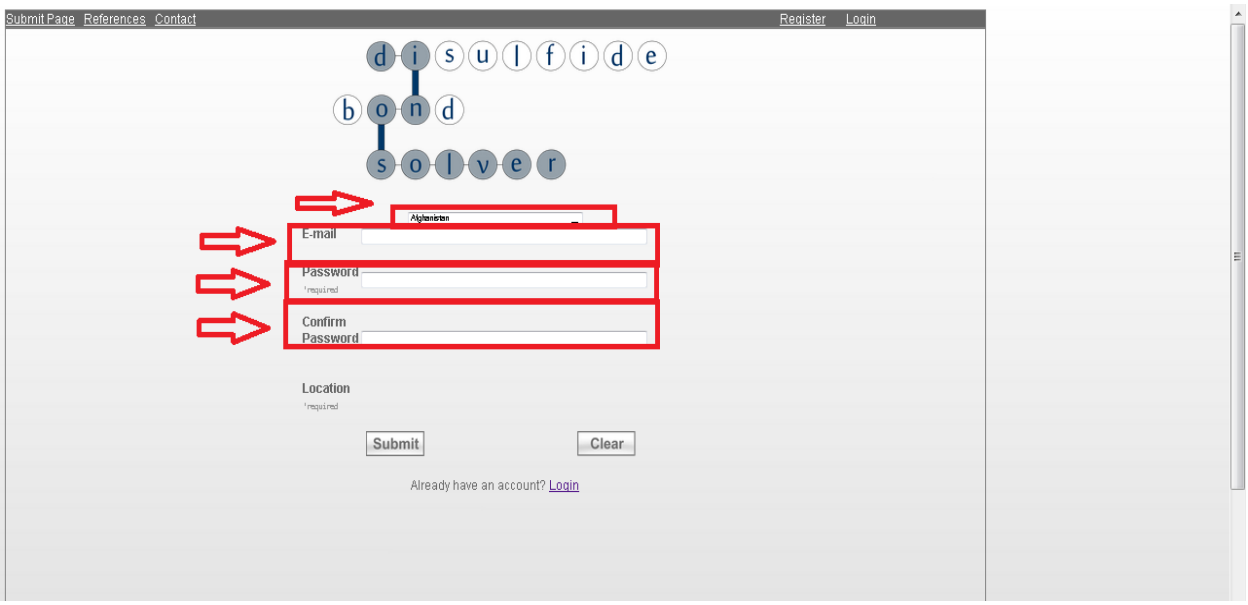

Figure 12. Register User Country Drop Down Box

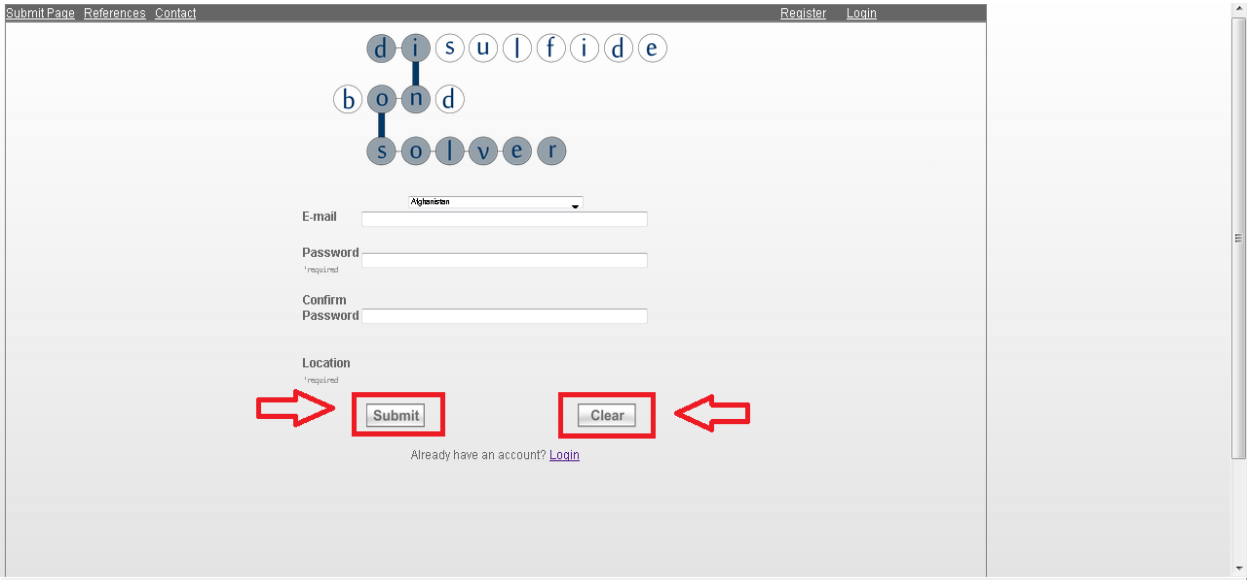

Figure 13. Register User Submit and Clear Buttons

User Login (Sybil Melton)

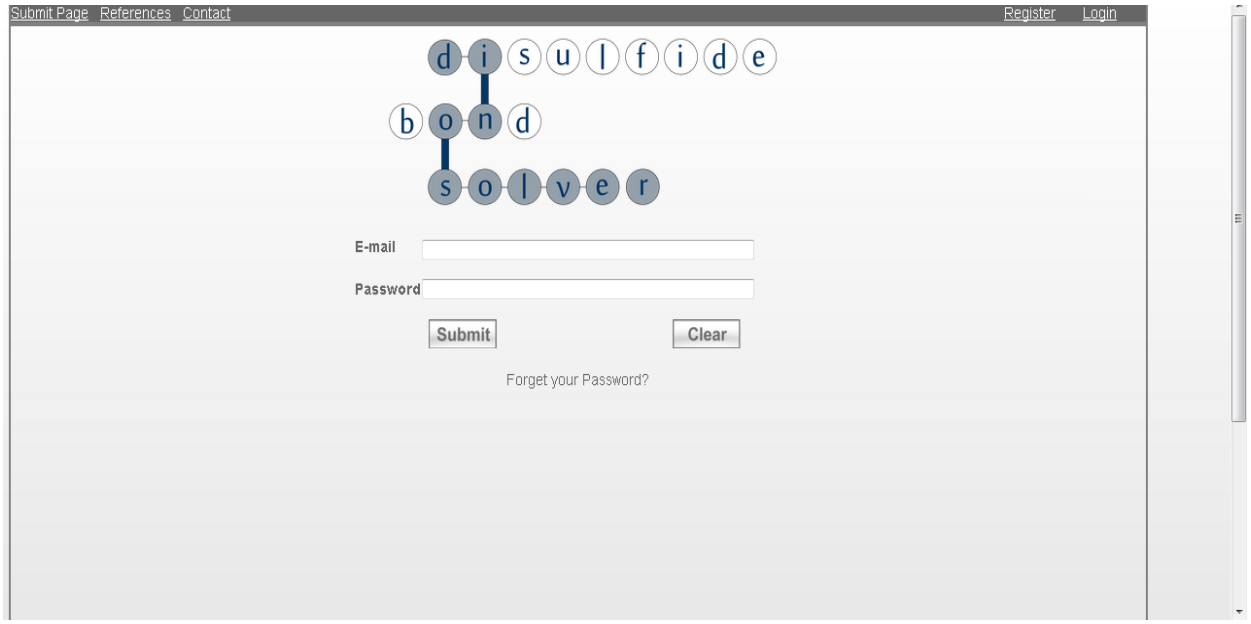

Figure 14. User Login Screen

To log into Dinosolve follow these steps:

1. Enter your email into the text box.

2. Enter your password into the password text box.

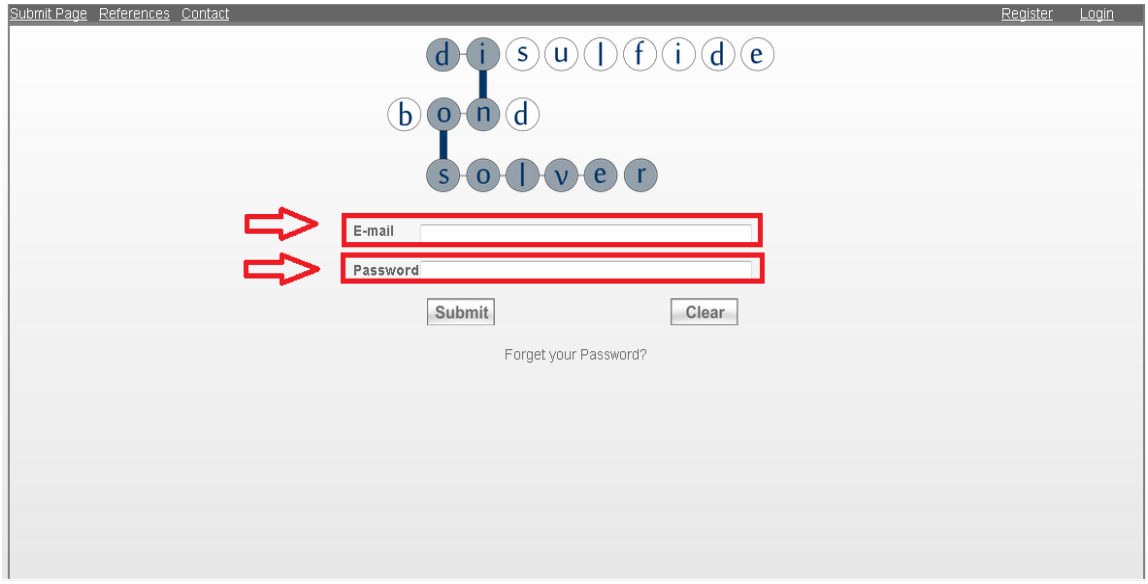

Figure 15. User Email and Password Text Fields

3. Click the Submit button.

To clear your inputs from the login page, click the Clear button.

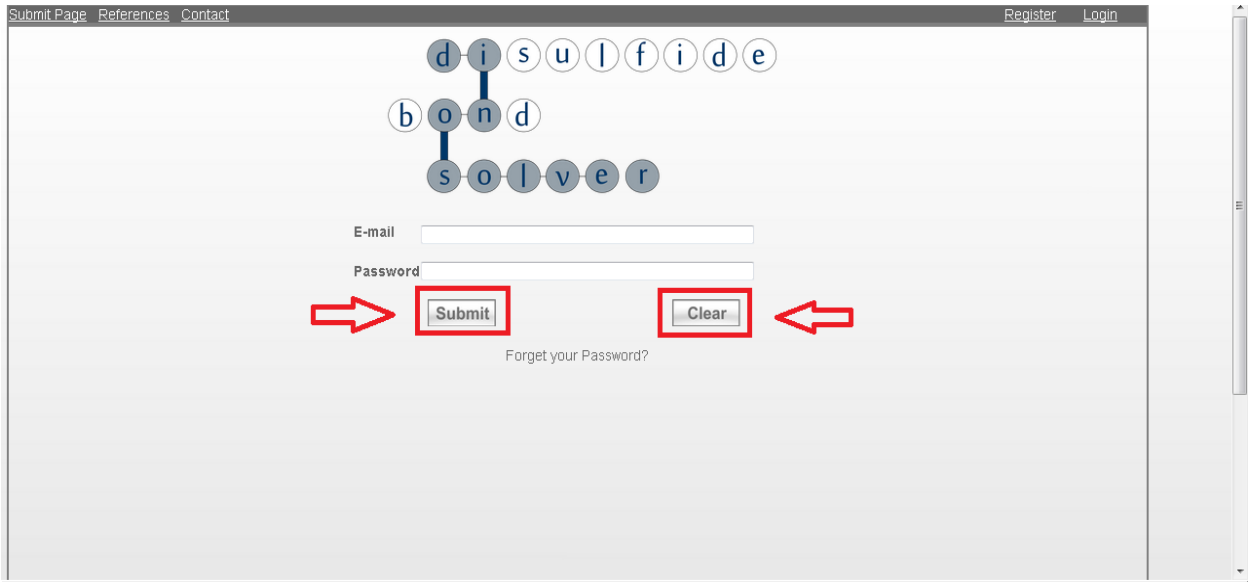

Figure 16. Login page Submit and Clear

If you forget your password, click the “Forgot your Password?” Link. It will bring you to the following page.

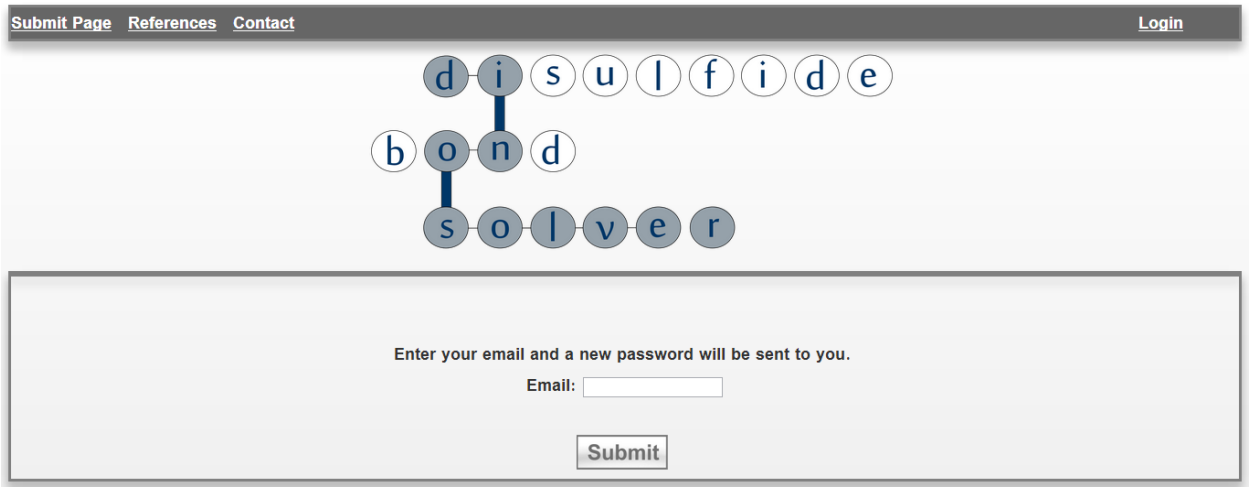

Figure 17. Password Reset

To reset your password, follow these steps:

1. Enter your email that you used to register with Dinosolve.
2. Click the Submit button.

A randomly generated password will be emailed to the email address you registered with.

If you click submit without entering an email, you will see the following error message:

Email cannot be blank

If you click submit and enter the wrong email, you will see the following error message:

Email not found

If you click submit and you have used Dinosolve but have not registered, you will see the following error message:

Not a registered user.

Once successfully logged in, you will be directed to the user account page. This page provides you links to view your pending and completed submitted sequences and change your password.

To change your password, click the “Change Password” link. You will re-directed to the change password page.

<Need screen shot>

Enter your new password and click the Submit button. If your password is successfully changed, you will be redirected back to your account page. If the new password entered does not conform to the password requirements, you will see the following error message:

Password must be between 8 and 16 characters

To view your completed sequences, click the Completed tab.

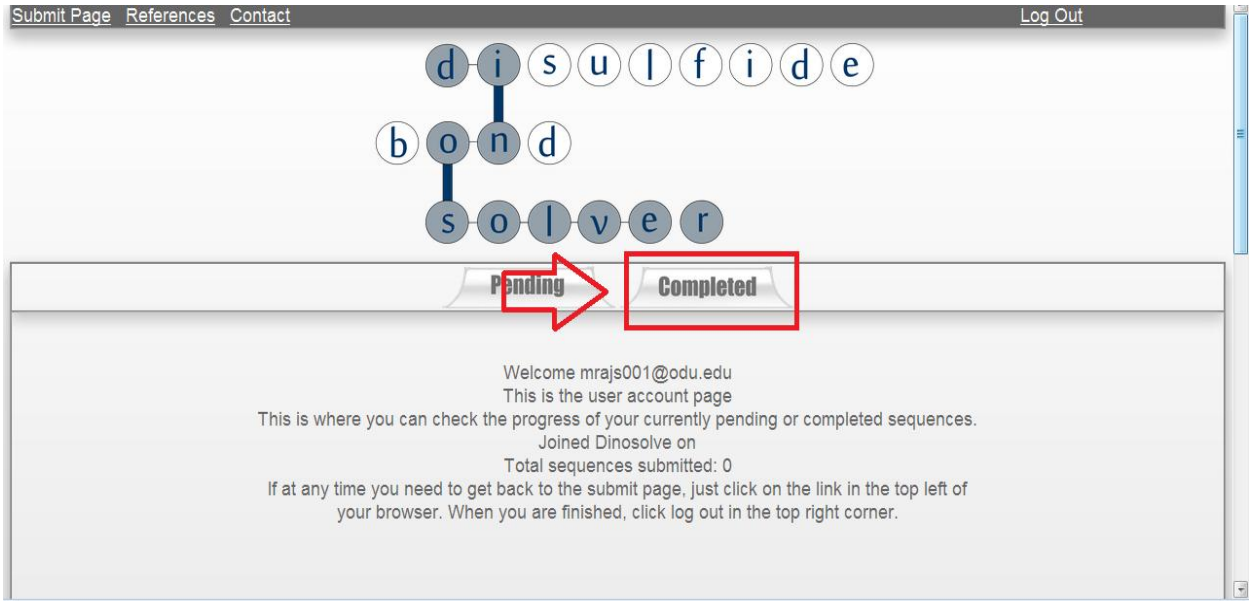
Submit Page
References
Contact
Log Out
disulfide
bond
solver
Pending
Completed
Welcome mrajs001@odu.edu
This is the user account page
This is where you can check the progress of your currently pending or completed sequences.
Joined Dinosolve on
Total sequences submitted: 0
If at any time you need to get back to the submit page, just click on the link in the top left of
your browser. When you are finished, click log out in the top right corner.

Figure 18. User Login Page Complete Tab

The Completed page shows you the title, sequence, connectivity state, bonding state, and submission time of the sequence. Completed sequences can be resubmitted if there is an algorithm update. To resubmit sequences, follow these steps:

1. Click the check box next to the sequence.
2. Click the Resubmit button.

An email will be sent to you with the results when the job is completed.

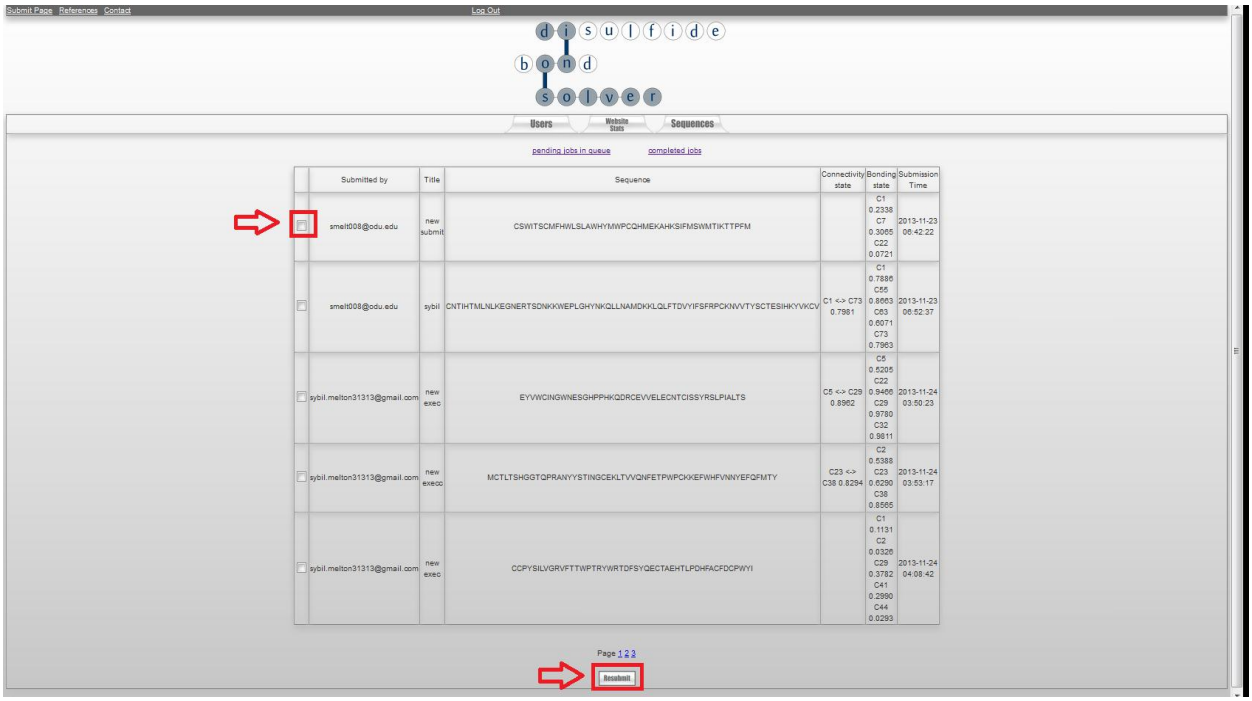

Figure 19. User Login Select Sequence and Resubmit Button

To view your sequences that have not been completed, click the Pending tab.

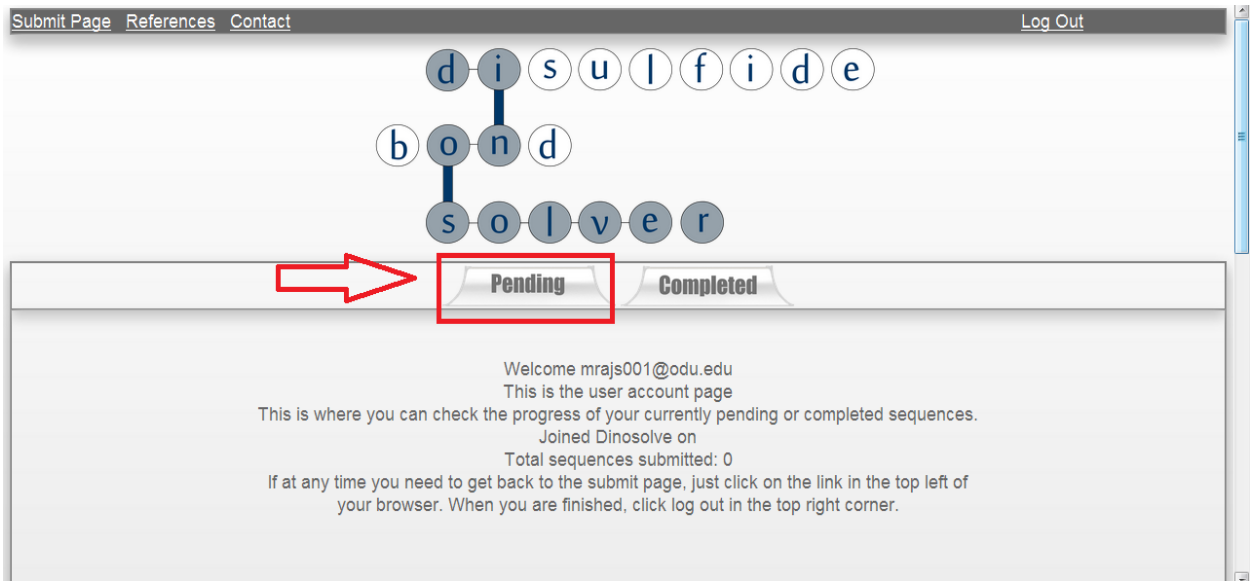
Submit Page References Contact Log Out
disulfide
bond
solver
Pending
Completed
Welcome mrajs001@odu.edu
This is the user account page
This is where you can check the progress of your currently pending or completed sequences.
Joined Dinosolve on
Total sequences submitted: 0
If at any time you need to get back to the submit page, just click on the link in the top left of your browser. When you are finished, click log out in the top right corner.

Figure 20. User Login Pending Tab

The pending sequence page will show you the title, sequence, and submission time.

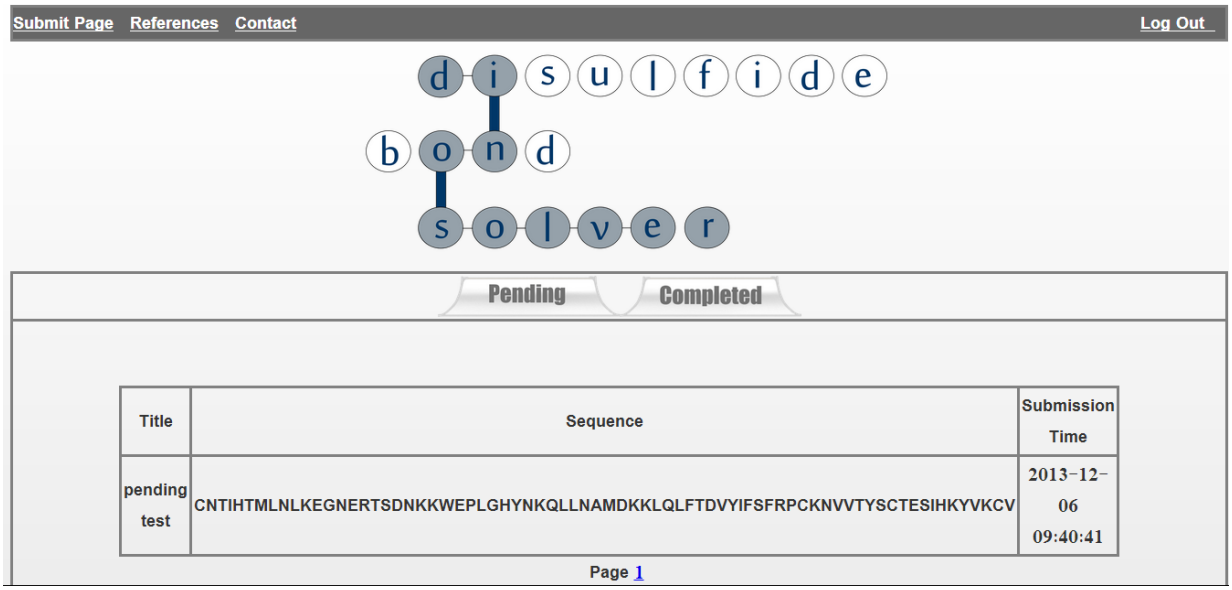

Figure 21. Pending Sequences

At any time if you wish to return to the Submit Page, view References, or contact Dinosolve administrators, links are available on the top left hand of the page.

Submit Page References Contact
Log Out
Pending
Completed
Welcome mrajs001@odu.edu
This is the user account page
This is where you can check the progress of your currently pending or completed sequences.
Joined Dinosolve on
Total sequences submitted: 0
If at any time you need to get back to the submit page, just click on the link in the top left of your browser. When you are finished, click log out in the top right corner.

Figure 22. User Home Page, Reference Contact Link

To logout of your account, the Log Out link is at the top right of the page.

Submit Page References Contact
Log Out
Pending
Completed
Welcome mrajs001@odu.edu
This is the user account page
This is where you can check the progress of your currently pending or completed sequences.
Joined Dinosolve on
Total sequences submitted: 0
If at any time you need to get back to the submit page, just click on the link in the top left of your browser. When you are finished, click log out in the top right corner.

Figure 23. User Logout Button

When you click Log Out, you will be automatically logged out and redirected to the logout page.

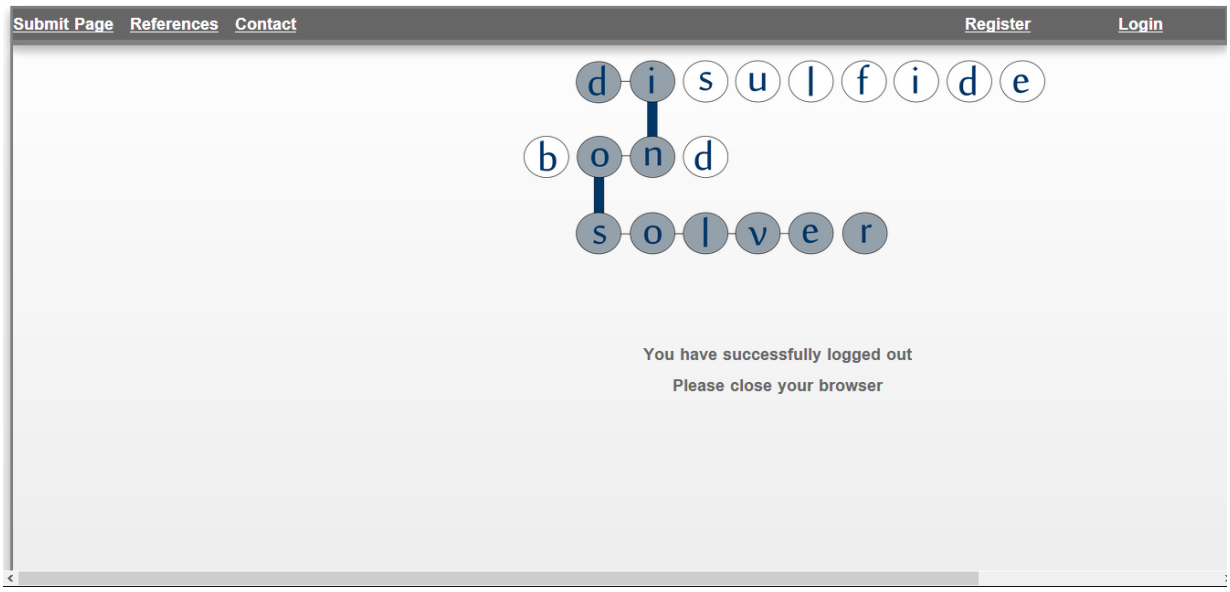

Figure 24. Logout Screen

Administrator Utilities Page (David Crook)

Main Page

The main page of the Administrator's page has 3 tabs (as shown in Figures 26, 29, and 32). The first tab is a tab labeled "Users". This button redirects you to the Users page, which will allow you to ban, search for, or change the password for a user. The second tab is a tab labeled "website stats". This tab will redirect you to a page he can use to view the total hits or hits by country for Dinosolve. The third tab is the Sequences tab. The sequences tab will redirect you to a page where you can view pending jobs in the queue or completed jobs currently stored in the database.

Users Page

The users page links to two pages that provide different functionality (Shown in figure 25). The first option on the left will redirect you to the "all users" version of the users page where it simply lists every user 10 at a time. The second option will let you search for a specific

user using their email address. On either version, you will be provided with a table of users. Each user on the table will have a checkbox next to them, along with their number of sequences personally submitted and whether or not that user is an admin. At the bottom of the table are numbers that redirect the user to more pages of users. Below the pages are the "Ban", "Set admin", and "Reset Password" buttons. The "ban" button will ban all of the users with a checked checkbox next to them. The "set admin" button lets you set all users currently checked to administrator status or vice versa. The "reset password" button will let you reset the password of the selected users (shown in Figure 29). The users page is on the search users version by default.

Search Users Page

The search users page is the search version of the users page. It is made for when you need to find a specific user. The search is performed by entering an email address using the field after "search users" and clicking the submit button (shown in Figure 27). After searching for a user, if there is a person with the email address being searched, the table will update with the user and his specifics in it. If there is not a person with the email address being searched currently registered, the user will not show up.

All Users Page

The all users page will show all users 10 at a time, divided by clickable page numbers.

Website Stats page

This page will show you the current hits of the Dinosolve website in total and by city (shown in Figure 30). Above the table are total pageviews and total unique visits. The table itself

will show each country in the first column and its individual pageviews and unique visits in the second column.

Administrator Sequences Page

The administrator sequences page is where you can interact with jobs currently pending or stored on the server. There are two different versions of this page. This page starts on the "Pending jobs in the queue" page by default.

Pending jobs administrator page

This page will show you the jobs currently in the queue. The jobs are shown in a table where their title, sequence, connectivity state, bonding state, submission time, and a checkbox are shown in different columns. Below the table is a "delete" button that when pressed will delete all of the checked sequences from the queue.

Completed jobs administrator page

The completed jobs administrator page will show you all of the jobs that were completed and stored. Each of the jobs will be shown in a table where the email address of the user who submitted it, title, sequence, results, submission time, and a checkbox are shown in different columns. Below the table is a "resubmit button" that will resubmit all checked sequences back into the queue for parsing.

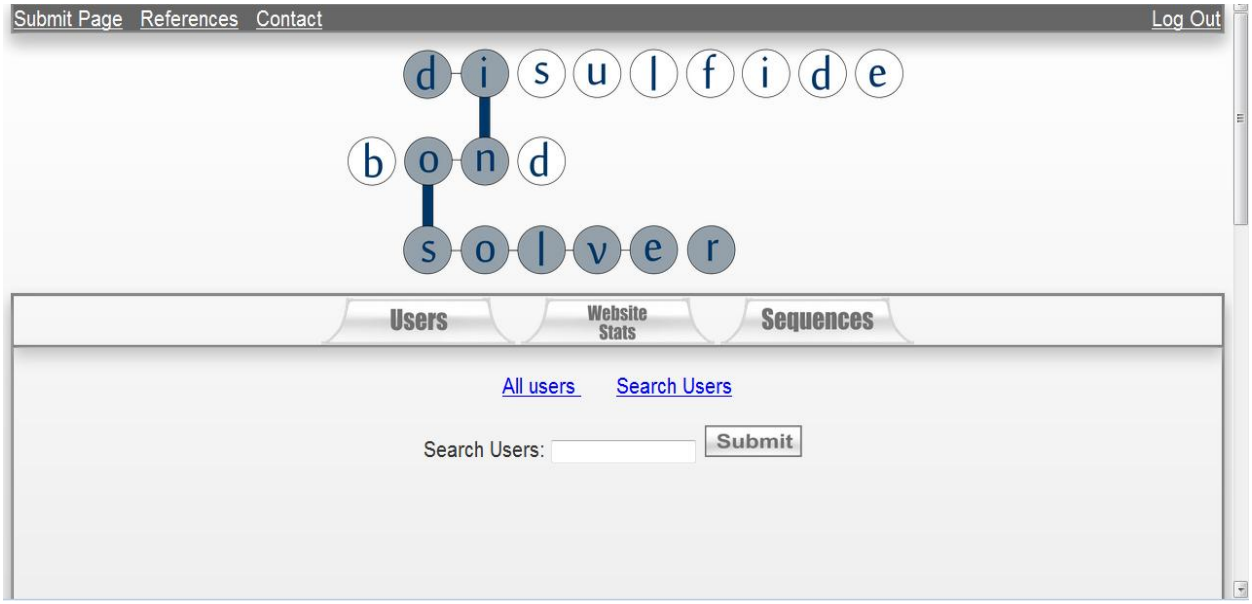

Figure 25. Administrator Page

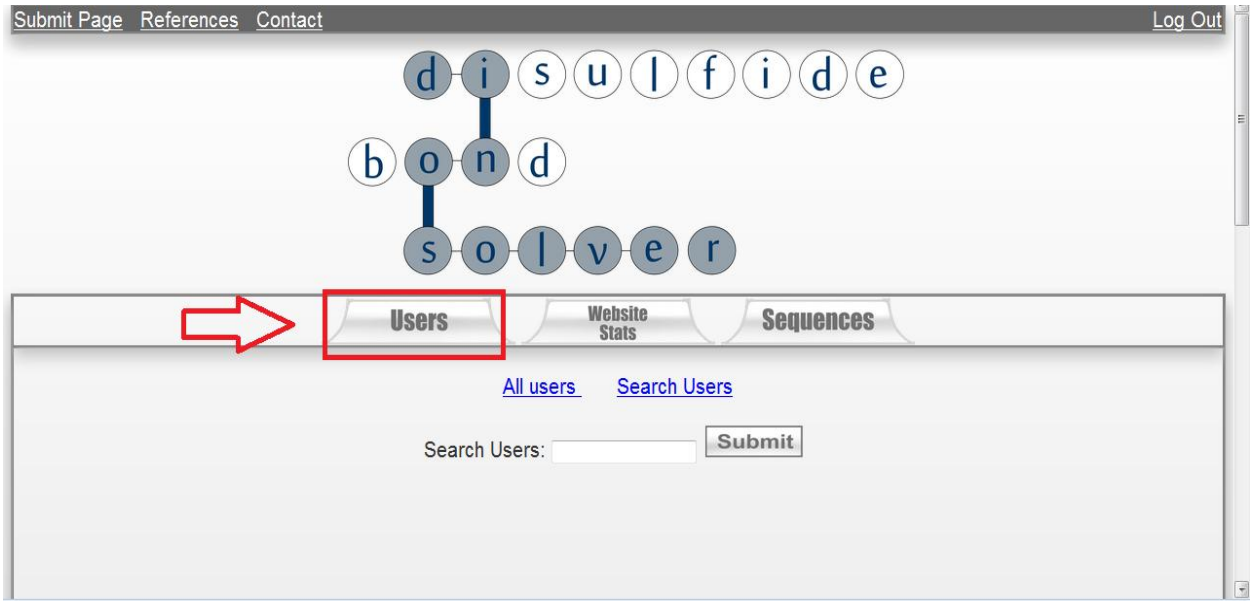

Figure 26. Administrator Users Button

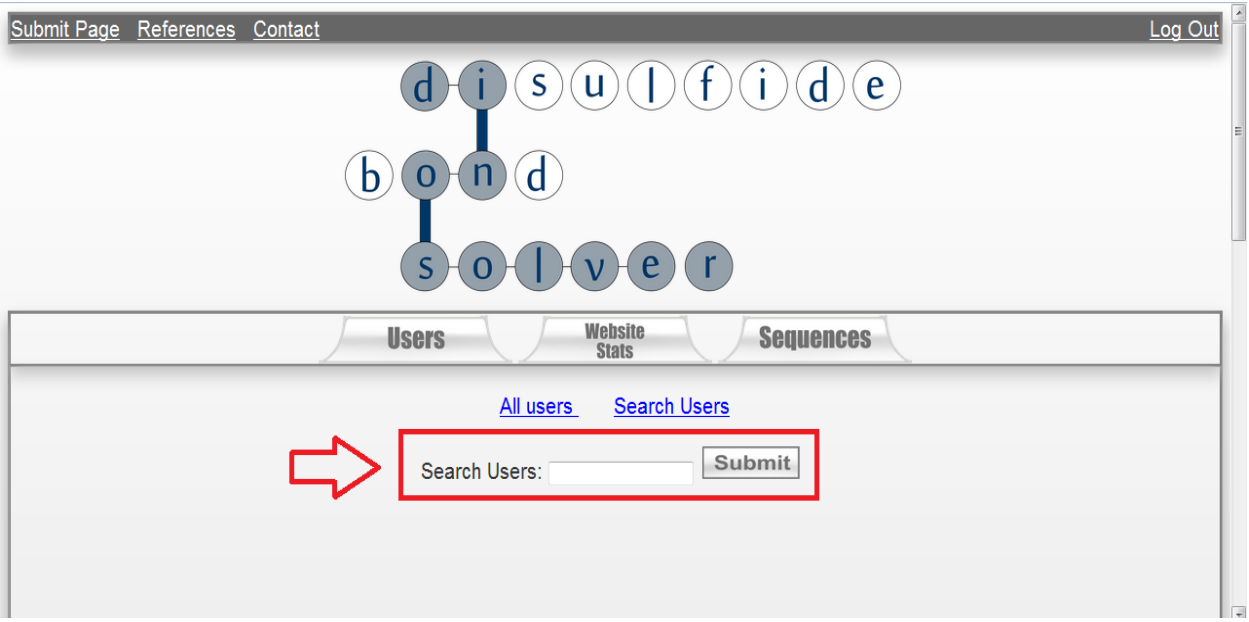

Figure 27. Administrator User Search

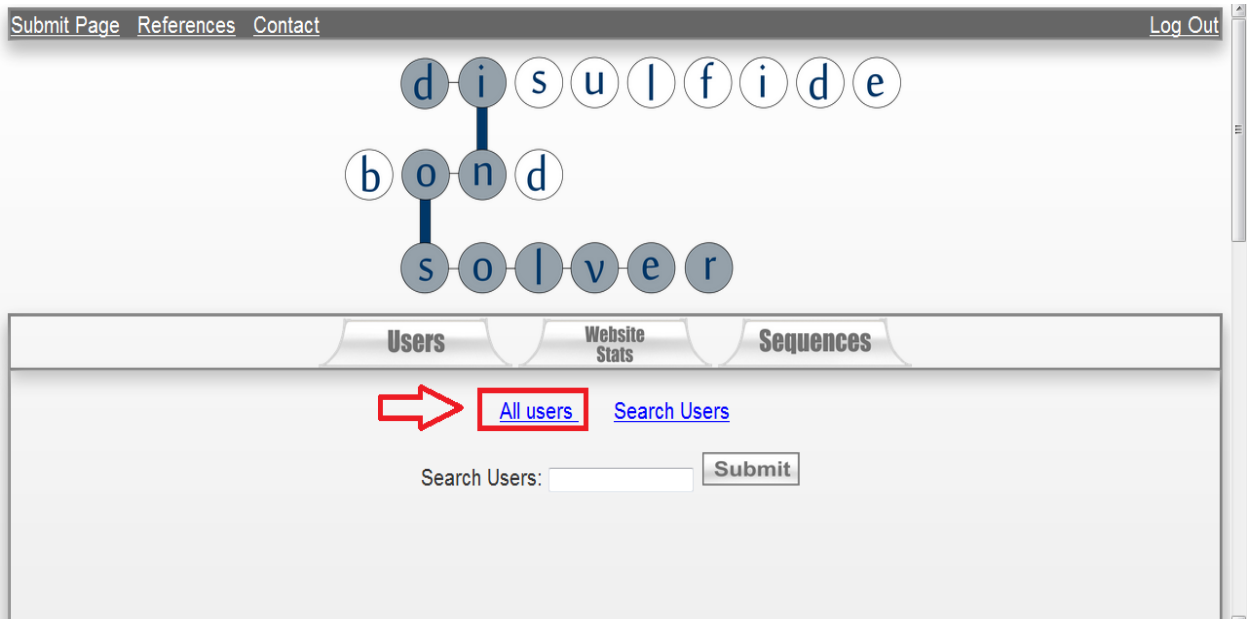

Figure 28. Administrator Search All Users

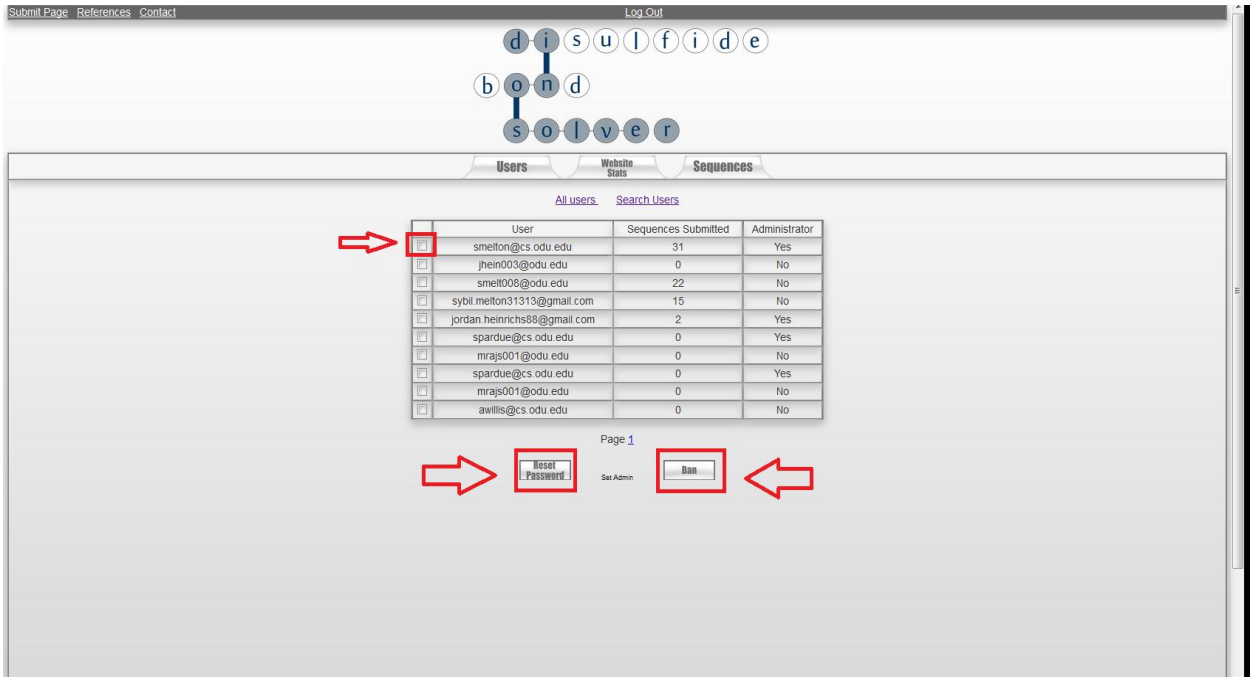

Figure 29. Administrator Select User Reset Password, or Ban

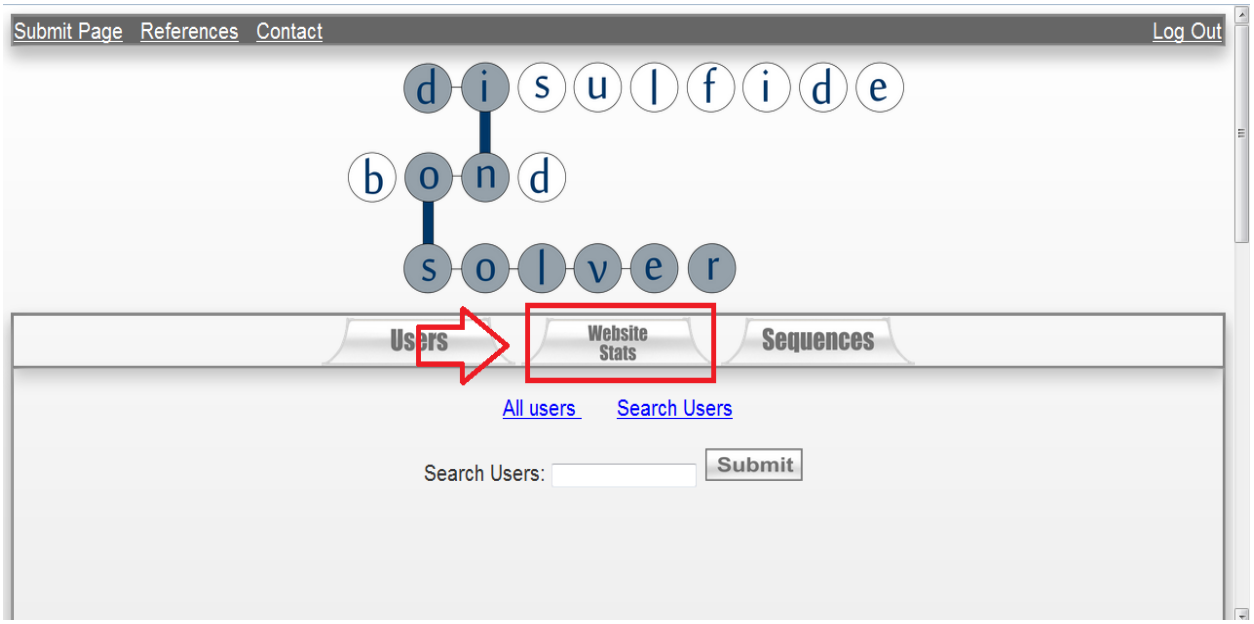

Figure 30. Website Stats Tab

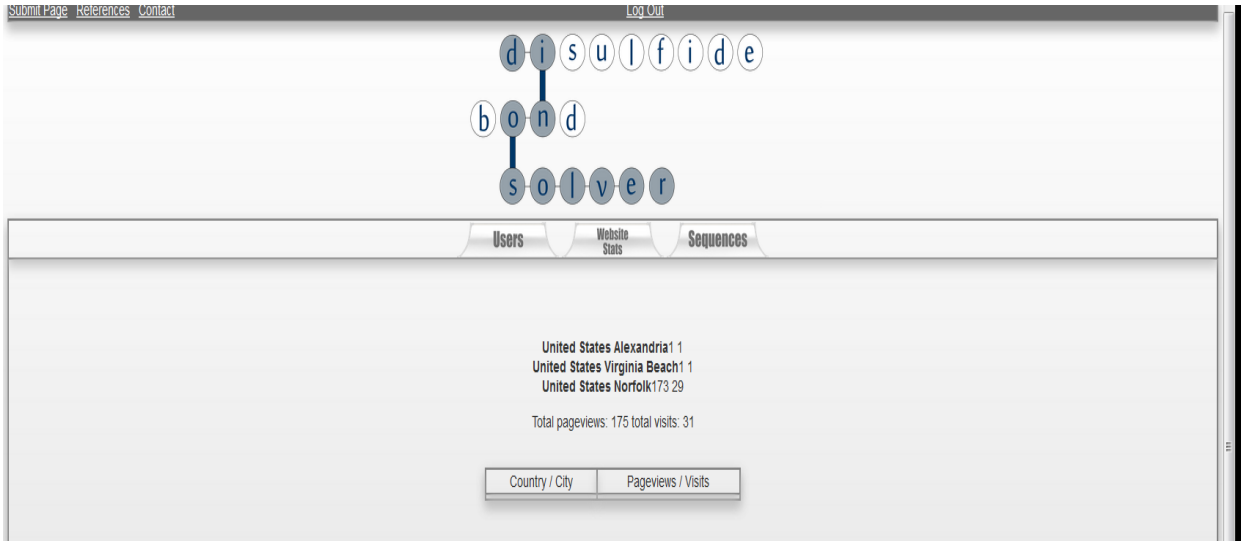

Figure 31. Website Statistics

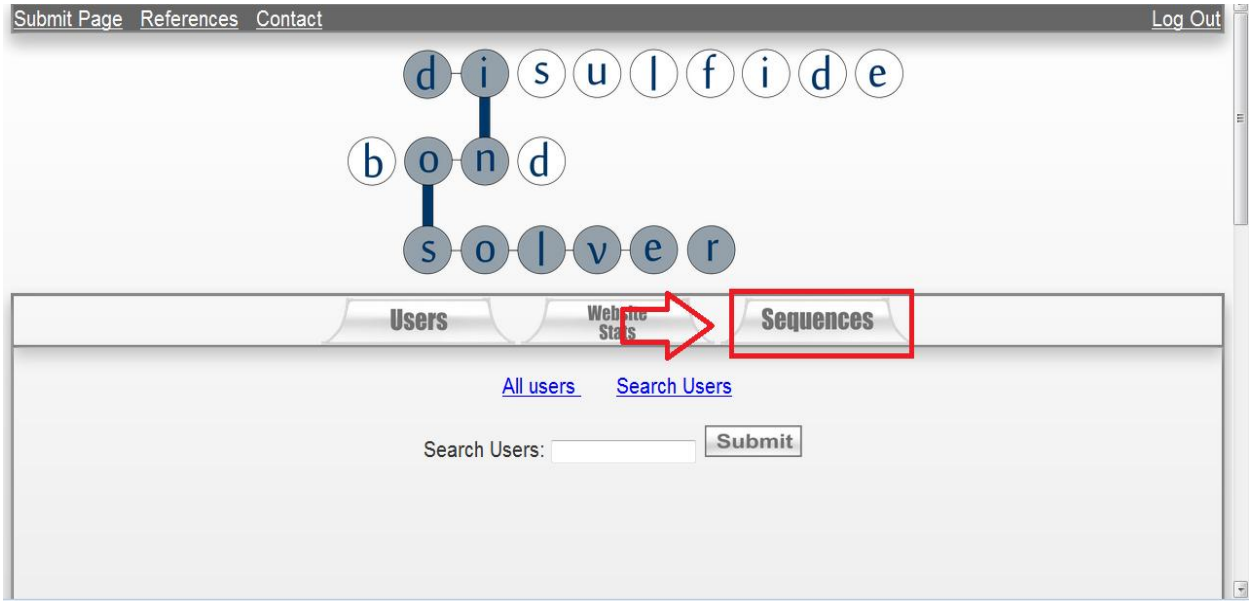

Figure 32. Administrator Sequences Tab